

US EPA ARCHIVE DOCUMENT

TABLE A-3-51

## CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	350.59
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	314.6
$V_p$ (atm)	$V_p$ value cited in Howard (1989-1993).	--	1.32E-03 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in Howard (1989-1993).	--	5.00E+00
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.26E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.82E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.42E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	1.82E+05
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.79E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.79E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.35E+03

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## CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	7.18E+02
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.61E+03
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.46E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.53E-02
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.53E-02
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.42E-01

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CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (continued)</b>			
$Bv_{forage}$ ( $\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}$ )	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.42E-01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.45E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.57E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	5.53E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.45E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.61E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.81E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.03E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-02
$Inhalation URF$ ( $\mu\text{g/m}^3$ ) <sup>-1</sup>	--	C-2-1	ND

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Parameter	Reference and Explanation	Equations	Value
Health Benchmarks (continued)			
Inhalation CSF (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:  
 NA = Not applicable  
 ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-52

## CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (7440-47-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	52
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	2,173.1
$V_p$ (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
$S$ (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
$H$ (atm·m <sup>3</sup> /mol)	$H$ value is assumed to be zero, because the $V_p$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.01E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	B-4-20	4.63E-05
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	$Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0

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## CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (7440-47-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND
$F_v$ (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{rootveg}$ .	B-2-10	4.50E-03
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{ag}$ (fruits). $Br_{ag}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $B_v$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoeren, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	4.88E-03
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $B_v$ values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{forage}$ .	B-3-8	7.50E-03
$Br_{grain}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{grain}$ value was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative growth as recommended by Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{grain}$ .	B-3-8	4.50E-03
$B_{vag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

TABLE A-3-52

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (7440-47-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	1.5E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	5.5E-03
$Ba_{pork}$ (day/kg FW)		B-3-12	ND
$Ba_{eggs}$ (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
$BCF_{fish}$ (L/kg FW tissue)	Geometric mean value obtained from Thompson, Burton, Quinn, and Ng (1972) for freshwater and marine fish.	B-4-26	2.83E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	$RfD$ value cited in U.S. EPA (1995c) for Chromium (III).	C-1-8	1.0E+00
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.5E+00
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-53

## CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	52
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	2,173.0
$V_p$ (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
$S$ (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
$H$ (atm·m <sup>3</sup> /mol)	$H$ value is assumed to be zero, because the $V_p$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.36E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.58E-05
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	$Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

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## CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$F_v$ (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjöreen, and Shor (1984). $Br$ values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjöreen, and Shor (1984) were used for $Br_{rootveg}$ .	B-2-10	4.50E-03
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjöreen, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjöreen, and Shor (1984) were used for $Br_{ag}$ (fruits). $Br_{ag}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjöreen, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $B_v$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjöreen, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	4.88E-03
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was obtained from Baes, Sharp, Sjöreen, and Shor (1984). $B_v$ values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjöreen, and Shor (1984) were used for $Br_{forage}$ .	B-3-8	7.50E-03
$Br_{grain}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{grain}$ value was obtained from Baes, Sharp, Sjöreen, and Shor (1984). $Br$ values for nonvegetative growth as recommended by Baes, Sharp, Sjöreen, and Shor (1984) were used for $Br_{grain}$ .	B-3-8	4.50E-03
$B_{vag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

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## CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $(\frac{\mu\text{g/g } DW \text{ plant}}{\mu\text{g/g air}})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	1.5E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	5.5E-03
$Ba_{pork}$ (day/kg FW)	--	B-3-12	ND
$Ba_{egg}$ (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ values were obtained from U.S. EPA (1995b) for all metals, except lead and mercury.	B-4-26	3.0E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	$RfD$ value cited in U.S. EPA (1997b) for Chromium (VI).	C-1-8	5.0E-03
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	Calculated based on <i>Inhalation URF</i> using inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-1-7	4.1E+01
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.8E-02
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	<i>Inhalation URF</i> value cited in U.S. EPA (1997b) for Chromium (VI).	C-2-1	1.2E-02
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	<i>Inhalation CSF</i> value cited in U.S. EPA (1997c) for Chromium (VI).	C-2-2	4.1E+01

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-54

## CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	228.28
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	527.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.03E-11 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.94E-03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.21E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.48E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	6.21E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.48E+05
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.97E+05
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.97E+03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.23E+04
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.19E+04

TABLE A-3-54

## CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.53E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.761
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.10E+03
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.05E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.866E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.866E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.97E+04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.97E+04

TABLE A-3-54

CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.355E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.377E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.67E-02
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.35E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.09E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	6.03E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	Calculated by multiplying the $Oral\ CSF$ for Benzo(a)pyrene by the relative potency factor for chrysene of 0.001 (U.S.EPA 1993e)	C-1-7	7.3E-03
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.1E-06
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-55

## CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	108.13
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	284.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	1.90E-04 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	2.30E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.93E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.93E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.30E-06
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b)	--	9.10E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.78E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.78E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.58E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.91E+00



TABLE A-3-55

## CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	8.72E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.38E+01
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.89E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.86E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.86E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	7.64E+00
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	7.64E+00



TABLE A-3-55

## CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.23E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.29E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.77E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.23E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.86E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.81E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.8E+00
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable  
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-56

## CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	108.13
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	303.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.16E-04 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.77E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.62E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.88E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.41E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.05E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.34E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.34E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.0E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.14E+00

TABLE A-3-56

## CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.47E+01
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.75E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.63E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.63E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.89E+00
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.89E+00

TABLE A-3-56

CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	8.34E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.64E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.19E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	8.34E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.08E-06
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.02E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.80E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable  
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-57

## CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	108.13
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	308.6
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	1.70E-04 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	2.30E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.99E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.93E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.30E-06
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b).	--	8.70E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.61E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.61E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.46E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.84E+00

TABLE A-3-57

## CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.79E+02
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.35E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.94E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.93E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.93E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	8.13E+00
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	8.13E+00

TABLE A-3-57

## CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.91E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.19E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.65E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.91E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.73E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.75E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	5.00E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.80E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-58

## CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	120.19
$T_m$ (K)	U.S. EPA (1995b)	--	177
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	6.00E-03 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	5.60E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.29E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.50E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.83E-06
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b)	--	4.10E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	9.31E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.31E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.98E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.72E+02



TABLE A-3-58

## CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.16E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.47E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.58E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.16E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.16E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.06E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.06E-02

TABLE A-3-58

## CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.26E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.03E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.25E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.26E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	8.13E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.28E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	NA
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	4.00E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	NA

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

**TABLE A-3-59**  
**CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S.EPA (1992a)	--	26.017
$T_m$ (K)	--	--	ND
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.82E-02 at 25°C (solid)
$S$ (mg/L)	--	--	ND
$H$ (atm·m <sup>3</sup> /mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.48E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	2.10E-05
$K_{ow}$ (unitless)	--	--	ND
$K_{oc}$ (mL/g)	--	--	ND
$Kd_s$ (cm <sup>3</sup> /g)	--	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	ND
$Kd_{sw}$ (L/Kg)	--	B-4-16; B-4-18; B-4-24	ND
$Kd_{bs}$ (cm <sup>3</sup> /g)	--	B-4-16; B-4-25	ND
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be zero due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0

**TABLE A-3-59**  
**CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	--	B-2-10	ND
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	--	B-2-9	ND
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	--	B-3-9	ND
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	--	B-2-8	ND
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	--	B-3-8	ND
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	--	B-3-11	ND
$Ba_{beef}$ (day/kg FW)	--	B-3-10	ND
$Ba_{pork}$ (day/kg FW)	--	B-3-12	ND
$Ba_{eggs}$ (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—see Appendix A-3.	B-4-26	6.33E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	ND

**TABLE A-3-59**  
**CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)**

Parameter	Reference and Explanation	Equations	Value
<i>BSAF<sub>fish</sub></i> (unitless)	--	B-4-28	NA
<b>Health Benchmarks (Continued)</b>			
<i>RfD</i> (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
<i>Oral CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
<i>RfC</i> (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E-02
<i>Inhalation URF</i> (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
<i>Inhalation CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable  
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

**TABLE A-3-60**  
**CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	320.05
$T_m$ (K)	Montgomery and Welkom (1991)	--	380.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.14E-09 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.33E-02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.98E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.69E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.76E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.32E+06
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	4.58E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.58E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.44E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.83E+03

**TABLE A-3-60**  
**CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.34E-02
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.925
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.20E+04
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.62E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.12E-02
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.12E-02
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.70E+04
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.70E+04

**TABLE A-3-60**  
**CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.05E-02
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.31E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.01E-02
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.05E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.62E-02
$BCF_{fish}$ (L/kg, FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.25E+05
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	2.40E-01
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	6.90E-05
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	2.40E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-61

## CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	319.03
$T_m$ (K)	Montgomery and Welkom (1991)	--	361.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	7.45E-09 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.92E-02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.24E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.70E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.78E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.80E+06
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	8.64E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.64E+06
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.48E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.46E+03

**TABLE A-3-61**  
**CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.34E-02
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.981
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.53E+04
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.77E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	9.37E-03
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	9.37E-03
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.08E+03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.08E+03

**TABLE A-3-61**  
**CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.43E-02
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.53E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	5.49E-02
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.43E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.58E-02
$BCF_{fish}$ (L/kg, FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.53E+05
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	3.40E-01
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from the $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	9.7E-05
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	3.40E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-62

## CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	354.49
$T_m$ (K)	Montgomery and Welkom (1991)	--	381.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.17E-10 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.41E-03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.37E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.48E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.48E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.17E+06
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.78E+05
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.78E+03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.08E+04
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.71E+04

**TABLE A-3-62**  
**CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.34E-02
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.852
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.10E+04
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.62E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.20E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.20E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for above ground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.03E+03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.03E+03

**TABLE A-3-62**  
**CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	9.33E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.95E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.57E-02
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	9.33E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.33E-02
$BCF_{fish}$ (L/kg, FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.30E+05
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	5.00E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	3.40E-01
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.80E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S.EPA (1997b)	C-2-1	9.70E-05
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997c)	C-2-2	3.40E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-63

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	278.34
$T_m$ (K)	Montgomery and Welkom (1991)	--	238.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.55E-08 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.08E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.43E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.38E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	7.86E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.25E+04
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.57E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.57E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.18E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.27E+01

TABLE A-3-63

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

Parameter	Reference and Explanation	Equations	Value
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.11E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.989
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.01E+03
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	6.43E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	7.24E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	7.24E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.16E+03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.16E+03



TABLE A-3-63

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.17E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.32E-03
<b>Biotransfer Factors for Animals (Continued)</b>			
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.60E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.17E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	1.04E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.58E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

**TABLE A-3-63**

**CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)**

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TABLE A-3-64

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (117-84-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	390.56
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	248.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.90E-09 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.00E+00
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.68E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.32E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.20E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.14E+09
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	9.03E+08
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.03E+06
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.78E+07
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.61E+07

TABLE A-3-64

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (117-84-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.55E+06
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	3.93E-01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.57E-04
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.57E-04
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.28E+08
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.28E+08

TABLE A-3-64

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (117-84-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.70E+01
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.37E+01
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	6.50E+01
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.70E+04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.24E+01
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.88E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997a)	C-1-8	2.00E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-65

## CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	304.36
$T_m$ (K)	Howard (1989-1993)	--	393.1
$V_p$ (atm)	$V_p$ value cited in Howard (1989-1993).	--	1.11E-07 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in Howard (1989-1993).	--	6.88E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.89E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.71E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.24E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.46E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.33E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.33E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.96E+02

TABLE A-3-65

## CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.31E+02
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	ND
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	2.06E+02
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.55E+00
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.43E-01
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.43E-01
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.31E+03



TABLE A-3-65

## CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

Parameter	Reference and Explanation	Equations	Value
$B_{V_{forage}}$ $\left( \frac{\mu\text{g/g } DW \text{ plant}}{\mu\text{g/g air}} \right)$	$B_{V_{forage}}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.31E+03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.13E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.62E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.96E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.13E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.28E-04
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). The geometric mean value was obtained from various literature sources (see Appendix A3.4).	B-4-26	4.63E+02
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were obtained from U.S. EPA (1995b). OR  Default $BAF$ value recommended for use by U.S. EPA (1995b), when literature data were not available	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	9.00E-04
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.15E-03
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:



## TABLE A-3-65

### CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-66

## CHEMICAL-SPECIFIC INPUTS FOR DIBENZ(A,H)ANTHRACENE (53-70-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	278.33
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	539.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.70E-14 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	6.70E-04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.12E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.80E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	6.01E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.53E+06
$K_{oc}$ (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	--	1.79E+06
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.79E+04
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.34E+05
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	7.16E+04

TABLE A-3-66

## CHEMICAL-SPECIFIC INPUTS FOR DIBENZ(A,H)ANTHRACENE (53-70-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.69E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.011
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.56E+04
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.43E-04
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.36E-03
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.36E-03
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.68E+07
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.68E+07

TABLE A-3-66

## CHEMICAL-SPECIFIC INPUTS FOR DIBENZ(A,H)ANTHRACENE (53-70-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.80E-02
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.86E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.07E-01
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.80E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (5.8/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	7.00E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.28E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	Calculated by multiplying the Oral CSF for Benzo(a)pyrene by the relative potency factor for Dibenz(a,h)anthracene of 1.0 (U.S.EPA 1993e).	C-1-7	7.30E+00
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.10E-03
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	7.30E+00

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

**TABLE A-3-66**

**CHEMICAL-SPECIFIC INPUTS FOR DIBENZ(A,H)ANTHRACENE (53-70-3)**

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TABLE A-3-67

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	236.36
$T_m$ (K)	Montgomery and Welkom (1991)	--	279.2
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	1.0E-03 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.20E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.97E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.79E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.79E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.19E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	9.47E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.47E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.10E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.79E+00

TABLE A-3-67

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.10E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.22E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.72E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.72E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	8.81E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	8.81E-02

TABLE A-3-67

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.74E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.50E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	6.65E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.74E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.34E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.54E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1996d)	C-1-8	5.70E-05
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-1-7	1.40E+00
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	2.00E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	4.00E-04
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1996d)	C-2-2	2.40E-03

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-68

## CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	208.3
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	252.1
$V_p$ (atm)	$V_p$ value cited in Montgomery and Weldom (1991).	--	2.00E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	3.44E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.21E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.96E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.05E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994g).	--	1.50E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	7.05E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.05E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.29E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.82E+00

TABLE A-3-68

## CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.73E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.45E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.14E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.14E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.59E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.59E-03

TABLE A-3-68

## CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.19E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.77E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.56E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.19E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.97E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980) (see Appendix A-3).	B-4-26	2.65E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	8.40E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.4E-05
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	8.4E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-69

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	147.01
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	256.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.79E-03 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.25E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.11E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.11E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.93E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.79E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.79E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.79E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.84E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.52E+01

TABLE A-3-69

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay and others (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.11E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.92E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.95E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.95E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.24E-01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.24E-01

TABLE A-3-69

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.21E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.00E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	8.48E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.21E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.53E-05
$BCF_{fish}$ (L/kg FW tissue)	BCFs were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.45E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	9.00E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	2.00E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii

TABLE A-3-70

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	147.01
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	297.86
$V_p$ (atm)	$V_p$ value cited in Howard (1989-1993).	--	3.03E-03 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in Howard (1989-1993).	--	6.88E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.11E+02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.14E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.85E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.39E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	8.03E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.03E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.02E+02



TABLE A-3-70

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.21E+02
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.28E+02
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.59E+00
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.53E-01
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.53E-01
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	8.02E-02

TABLE A-3-70

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ ( $\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}$ )	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	8.02E-02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.69E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.52E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.03E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.69E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	6.72E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.84E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	8.90E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.12E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

## TABLE A-3-70

### CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-71

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	147.01
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	326.6
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.39E-03 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.30E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.80E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.14E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.85E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	2.58E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.16E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.16E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.62E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.46E+01

TABLE A-3-71

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.05E+02
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.70E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.13E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.13E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	8.60E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	8.60E-02

TABLE A-3-71

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.05E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.49E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.86E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.05E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.12E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.31E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1996c)	C-1-8	2.30E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	2.40E-02
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	8.00E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	6.90E-03
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	2.40E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-72

## CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	253.13
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	405.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.89E-10 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.52E+00
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.08E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.28E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.48E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.76E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	8.70E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.70E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.52E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.48E+01



TABLE A-3-72

## CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.847
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.38E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.58E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.32E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.32E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.73E+04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.73E+04

TABLE A-3-72

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.99E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	9.44E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.14E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.99E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	7.45E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.07E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	NA
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	4.50E-01
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	NA
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	1.30E-04
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral CSF$ assuming route-to-route extrapolation.	C-2-2	4.50E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-73

## CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	120.92
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	115.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	6.40E+00 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	3.0E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.58E+00
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.77E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.00E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.44E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	6.85E+0
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.85E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.14E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.74E+00

TABLE A-3-73

## CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.70E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.48E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.19E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.19E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.33E-06
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.33E-06

TABLE A-3-73

## CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.15E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.63E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	4.40E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.15E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	2.87E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.58E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-01
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	2.00E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-74

## CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	98.97
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	175.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.0E-01 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	5.16E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.75E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.42E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.05E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	6.20E+01
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	5.30E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.30E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.98E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.12E+00



TABLE A-3-74

## CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.643
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.19E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.24E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{sg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.56E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.56E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	7.88E-04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	7.88E-04



TABLE A-3-74

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.93E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.56E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.89E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.92E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	1.23E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.36E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.00E-01
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-1-7	9.1-E-02
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	5.00E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.60E-05
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral CSF$ assuming route-to-route extrapolation.	C-2-2	9.1-E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-75

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (107-06-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	98.96
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	233.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.07E-01 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	8.31E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.27E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.19E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.10E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.90E+01
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.96E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.96E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.47E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	7.83E-01

TABLE A-3-75

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (107-06-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.41E+00
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	4.81E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.53E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.53E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.58E-03
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.58E-03

TABLE A-3-75

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (107-06-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.30E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.28E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	8.82E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.30E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.75E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	7.61E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1996b)	C-1-8	2.90E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	9.10E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.00E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	2.60E-05
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-2-2	9.10E-02

Note:

NA= Not applicable  
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-76

## CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	96.95
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	150.6
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	7.88E-01 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.0E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.55E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.53E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.09E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.32E+02
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.50E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.50E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.88E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.60E+00

TABLE A-3-76

## CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.63E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.50E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.30E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.30E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.98E-04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.98E-04

TABLE A-3-76

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.05E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.32E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	4.01E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.05E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	2.62E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.41E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	9.00E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	6.00E-01
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.20E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	5.00E-05
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997c)	C-2-2	1.80E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-77

## CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Howard (1989-1993)	--	96.94
$T_m$ (K)	Howard (1989-1993)	--	192.6
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.30E-01 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.94E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.51E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.36E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.13E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	9.60E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.98E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.98E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.73+01

TABLE A-3-77

## CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.99E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.41E+01
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.38E+00
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.77E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.77E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.60E-03

TABLE A-3-77

## CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ ( $\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}$ )	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.60E-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.63E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.41E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.92E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.63E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.90E-06
$BCF_{fish}$ (unitless, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.89E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

## TABLE A-3-77

### CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-78

## CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	96.95
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	223.7
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	4.63E-01 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	6.03E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.44E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.16E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	9.75E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	9.60E+01
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.80E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.80E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.85E+00

TABLE A-3-78

## CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.52E+00
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.41E+01
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.71E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.77E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.77E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.70E-04

TABLE A-3-78

## CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

Parameter	Reference and Explanation	Equations	Value
$B_{V_{forage}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$B_{V_{forage}}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.70E-04
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.63E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.41E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.92E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.63E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.90E-06
<b>Biotransfer Factors for Animals (Continued)</b>			
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.89E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:



## TABLE A-3-78

### CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-79

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

Parameter	Reference and Explanation	Equations	Value																														
Chemical/Physical Properties																																	
$MW$ (g/mole)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	163.01																														
$T_m$ (K)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	318.1																														
$Vp$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	7.21E-06 at 25°C (solid)																														
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	4.93E+03																														
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.38E-07																														
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.69E-02																														
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.79E-06																														
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.09E+03																														
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	<table><tr><th>pH</th><th><math>K_{oc}</math></th></tr><tr><td>1</td><td>159.0</td></tr><tr><td>2</td><td>159.0</td></tr><tr><td>3</td><td>159.0</td></tr><tr><td>4</td><td>159.0</td></tr><tr><td>5</td><td>158.8</td></tr><tr><td>6</td><td>156.8</td></tr><tr><td>7</td><td>139.6</td></tr><tr><td>8</td><td>67.31</td></tr><tr><td>9</td><td>12.75</td></tr><tr><td>10</td><td>3.50</td></tr><tr><td>11</td><td>2.51</td></tr><tr><td>12</td><td>2.41</td></tr><tr><td>13</td><td>2.40</td></tr><tr><td>14</td><td>2.40</td></tr></table>	pH	$K_{oc}$	1	159.0	2	159.0	3	159.0	4	159.0	5	158.8	6	156.8	7	139.6	8	67.31	9	12.75	10	3.50	11	2.51	12	2.41	13	2.40	14	2.40
pH	$K_{oc}$																																
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11	2.51																																
12	2.41																																
13	2.40																																
14	2.40																																
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.40E+00																														

TABLE A-3-79

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.05E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.58E+00
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.68E+01
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	4.07E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.82E-01
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.82E-01

TABLE A-3-79

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

Parameter	Reference and Explanation	Equations	Value
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.01E+02
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.01E+02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	8.62E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.73E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.30E-05
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	8.62E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.15E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.19E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-79

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

Parameter	Reference and Explanation	Equations	Value
<b>Health Benchmarks</b>			
<i>RfD</i> (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-03
<i>Oral CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
<i>RfC</i> (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-02
<i>Inhalation URF</i> (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
<i>Inhalation CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-80

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	112.99
$T_m$ (K)	Montgomery and Welkom (1991)	--	172.7
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.66E-02 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.68E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.81E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.21E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.71E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.78E+02
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	4.70E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.70E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.53E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.88E+00

TABLE A-3-80

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

Parameter	Reference and Explanation	Equations	Value
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.96E-01
<b>Chemical/Physical Properties (Continued)</b>			
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.89E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_{ds}$ value provided in this table (see section A3.4.2 of Appendix A-3)	B-2-10	4.01E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.94E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.94E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.96E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.96E-03



TABLE A-3-80

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.41E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.47E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	5.41E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.41E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	3.53E-06
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were obtained from U.S. EPA (1995b).	B-4-26	3.02E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1996c)	C-1-8	1.10E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c))	C-1-7	6.80E-02
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	4.00E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	1.90E-05
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral CSF$ assuming route-to-route extrapolation.	C-2-2	6.80E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-81

## CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,3-DICHLOROPROPENE (542-75-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	110.98
$T_m$ (K)	Montgomery and Welkom (1991)	--	189.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.11E-02 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.55E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.94E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.26E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.00E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	5.60E+01
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.70E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.70E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.03E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.08E+00

TABLE A-3-81

## CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,3-DICHLOROPROPENE (542-75-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.24E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.15E+01
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	4.25E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.78E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.78E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.38E-03
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.38E-03

TABLE A-3-81

## CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,3-DICHLOROPROPENE (542-75-6)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.45E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.41E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.70E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.45E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.11E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.25E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-1-7	1.8E-01
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	2.0E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997c)	C-2-1	3.70E-05
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	1.3E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-82

## CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	220.98
$T_m$ (K)	--	--	NA
$V_p$ (atm)	$V_p$ value cited in Howard (1989-1993).	--	6.93E-05 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in Howard (1989-1993).	--	1.6E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.57E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.32E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.33E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	2.69E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.85E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.85E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.38E+00

TABLE A-3-82

## CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	7.38E-01
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	1.49E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.24E+00
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.00E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.78
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.78
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.95-03

TABLE A-3-82

## CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

Parameter	Reference and Explanation	Equations	Value
$B_{V_{forage}}$ $(\frac{\mu\text{g/g } DW \text{ plant}}{\mu\text{g/g air}})$	$B_{V_{forage}}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.95-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.14E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.76E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	8.18E-07
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.14E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.33E-07
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	7.19E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
$Oral \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	2.9E-01
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	5.00E-04
$Inhalation \text{ URF}$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral \text{ CSF}$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	8.3E-05
$Inhalation \text{ CSF}$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral \text{ CSF}$ assuming route-to-route extrapolation.	C-2-2	2.9E-01

Note:

NA = Not applicable

ND = No data available



## TABLE A-3-82

### CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-83

## CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	380.93
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	449.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a)	--	1.72E-12 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a)	--	1.87E-01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.51E-09
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.36E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	4.29E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.86E+05
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.55E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.55E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.91E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.02E+03

TABLE A-3-83

## CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	2.34E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.083
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.66E+03
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.04E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.49E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.49E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for above ground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.50E+06
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.50E+06

TABLE A-3-83

## CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.48E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.67E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	5.65E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.48E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.68E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.86E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	5.00E-05
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	1.60E+01
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.80E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S.EPA (1997b)	C-2-1	4.60E-03
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997c)	C-2-2	1.6-E+01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

**TABLE A-3-83**

**CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)**

TABLE A-3-84

## CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	222.24
$T_m$ (K)	Montgomery and Welkom (1991)	--	232.6
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.17E-06 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	8.80E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.48E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.56E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.35E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.73E+04
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	8.20E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.20E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.15E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.28E+00
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.52E+00

TABLE A-3-84

## CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

Parameter	Reference and Explanation	Equations	Value
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.12E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	7.46E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.06E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.06E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.42E+03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.42E+03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.17E-04



TABLE A-3-84

## CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.87E-04
<b>Biotransfer Factors for Animals (Continued)</b>			
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	8.31E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.17E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	5.42E-04
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.45E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.00E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.80E+00
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-85

## CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	194.19
$T_m$ (K)	Montgomery and Welkom (1991)	--	273.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.17E-06 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.19E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.01E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.96E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.13E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	4.30E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.66E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.66E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.00E+01

TABLE A-3-85

## CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.06E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.05E+01
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.95E+00
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.40E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.40E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.05E+01

TABLE A-3-85

## CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ ( $\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}$ )	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.05E+01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.42E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.08E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.31E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.42E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	8.53E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.03E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	1.00E+01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	NA
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E+01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	NA

Note:

NA = Not applicable

ND = No data available

## TABLE A-3-85

### CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-86

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

Parameter	Reference and Explanation	Equations	Value																																
Chemical/Physical Properties																																			
$MW$ (g/mole)	Moses (1978)	--	122.17																																
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	300.1																																
$Vp$ (atm)	$Vp$ value cited in U.S. EPA (1992a).	--	2.18E-07 at 25°C (solid)																																
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	6.25E+03																																
$H$ (atm·m³/mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.27E-09																																
$D_a$ (cm²/s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.84E-02																																
$D_w$ (cm²/s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.69E-06																																
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	2.29E+02																																
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	<table><tr><th>pH</th><th><math>K_{oc}</math></th></tr><tr><td>1</td><td>126.0</td></tr><tr><td>2</td><td>126.0</td></tr><tr><td>3</td><td>126.0</td></tr><tr><td>4</td><td>126.0</td></tr><tr><td>5</td><td>126.0</td></tr><tr><td>6</td><td>125.99</td></tr><tr><td>7</td><td>125.9</td></tr><tr><td>8</td><td>125.02</td></tr><tr><td>9</td><td>116.87</td></tr><tr><td>10</td><td>71.06</td></tr><tr><td>11</td><td>15.77</td></tr><tr><td>12</td><td>3.43</td></tr><tr><td>13</td><td>2.05</td></tr><tr><td>14</td><td></td></tr><tr><td></td><td>1.91</td></tr></table>	pH	$K_{oc}$	1	126.0	2	126.0	3	126.0	4	126.0	5	126.0	6	125.99	7	125.9	8	125.02	9	116.87	10	71.06	11	15.77	12	3.43	13	2.05	14			1.91
pH	$K_{oc}$																																		
1	126.0																																		
2	126.0																																		
3	126.0																																		
4	126.0																																		
5	126.0																																		
6	125.99																																		
7	125.9																																		
8	125.02																																		
9	116.87																																		
10	71.06																																		
11	15.77																																		
12	3.43																																		
13	2.05																																		
14																																			
	1.91																																		

TABLE A-3-86

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

Parameter	Reference and Explanation	Equations	Value
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.26E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.44E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.04E+00
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.997
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.16E+01
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.71E+01



TABLE A-3-86

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

Parameter	Reference and Explanation	Equations	Value
$Br_{ag}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}}\right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.68E+00
$Br_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}}\right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-8	1.68E+00
$Bv_{ag}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.27E+03
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.27E+03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.82E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.75E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	6.96E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.82E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.54E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.66E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-86

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

Parameter	Reference and Explanation	Equations	Value
<b>Health Benchmarks</b>			
<i>RfD</i> (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-02
<i>Oral CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
<i>RfC</i> (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-02
<i>Inhalation URF</i> (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
<i>Inhalation CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-87

## CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	244.28
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	410.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	3.30E-10 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	2.40E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.36E-10
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.38E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	5.60E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.46E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.65E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.65E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.74E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.46E+00

TABLE A-3-87

## CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.877
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.21E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	3.30E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.48E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.48E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.41E+04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.41E+04

TABLE A-3-87

## CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.13E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.62E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.96E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.13E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.28E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.40E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-1-7	1.40E-02
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	4.0E-03
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	1.40E-02

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-88

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	168.11
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	363
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994f).	--	4.0E-07 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994f).	--	5.4E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.25E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.18E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	9.15E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994f).	--	3.10E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.06E+01
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.06E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.55E+00
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.25E-01

TABLE A-3-88

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.58E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	4.64E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.32E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.32E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, C. Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.74E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.74E+01



TABLE A-3-88

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.46E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.79E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	9.43E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.46E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	6.15E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	7.40E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-89

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

Parameter	Reference and Explanation	Equations	Value																														
Chemical/Physical Properties																																	
$MW$ (g/mole)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	184.11																														
$T_m$ (K)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	385.1																														
$Vp$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.52E-07 at 25°C (solid)																														
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	5.8E+03																														
$H$ (atm·m³/mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.82E-09																														
$D_a$ (cm²/s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.73E-02																														
$D_w$ (cm²/s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.06E-06																														
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.30E+01																														
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	<table><tr><th>pH</th><th><math>\frac{K_{oc}}</math></th></tr><tr><td>1</td><td>0.80</td></tr><tr><td>2</td><td>0.79</td></tr><tr><td>3</td><td>0.72</td></tr><tr><td>4</td><td>0.38</td></tr><tr><td>5</td><td>0.08</td></tr><tr><td>6</td><td>0.02</td></tr><tr><td>7</td><td>0.01</td></tr><tr><td>8</td><td>0.01</td></tr><tr><td>9</td><td>0.01</td></tr><tr><td>10</td><td>0.01</td></tr><tr><td>11</td><td>0.01</td></tr><tr><td>12</td><td>0.01</td></tr><tr><td>13</td><td>0.01</td></tr><tr><td>14</td><td>0.01</td></tr></table>	pH	$\frac{K_{oc}}$	1	0.80	2	0.79	3	0.72	4	0.38	5	0.08	6	0.02	7	0.01	8	0.01	9	0.01	10	0.01	11	0.01	12	0.01	13	0.01	14	0.01
pH	$\frac{K_{oc}}$																																
1	0.80																																
2	0.79																																
3	0.72																																
4	0.38																																
5	0.08																																
6	0.02																																
7	0.01																																
8	0.01																																
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11	0.01																																
12	0.01																																
13	0.01																																
14	0.01																																
$Kd_s$ (cm³/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.0E-04 (at pH 7.0)																														

TABLE A-3-89

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	7.5E-04 (at pH 7.0)
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	4.0E-04 (at pH 7.0)
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.62E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.74E+00
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A3.4.2 in Appendix A-3).	B-2-10	9.74E+04
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.13E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.13E+00

TABLE A-3-89

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.80E+02
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.80E+02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.62E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.29E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.00E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.62E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	6.54E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	8.40E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND

TABLE A-3-89

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

Parameter	Reference and Explanation	Equations	Value
Inhalation CSF (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable  
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-90

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Howard (1989-1993)	--	182.14
$T_m$ (K)	Howard (1989-1993)	--	344
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.29E-07 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.85E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.46E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.09E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	7.86E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	9.90E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.10E+01
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.10E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.83E+00
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.04E+00

TABLE A-3-90

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/mL \text{ soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.43E+01
$Br_{root \text{ veg}}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.80E+01
$Br_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.72E+00
$Br_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.72E+00
$Bv_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.10E+01
$Bv_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.10E+01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.86E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.49E-06



TABLE A-3-90

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

Parameter	Reference and Explanation	Equations	Value
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.01E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.86E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.96E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	5.92E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, FW tissue)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1995d)	C-1-8	2.0E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	The $Oral CSF$ value represents a 2,4/2,6-Dinitrotoluene mixture (U.S. EPA 1997b).	C-1-7	6.8E-01
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral CSF$ assuming route-to-route extrapolation.	C-2-2	6.8E-01

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-91

## CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Howard (1989-1993)	--	182.15
$T_m$ (K)	Howard (1989-1993)	--	339
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	7.47E-07 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.05E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.30E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.11E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	7.76E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.70E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.19E+01
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.19E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.14E+00
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.68E+00

TABLE A-3-91

## CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.29E+01
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	3.08E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.15E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.15E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.41E+01
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.41E+01

TABLE A-3-91

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.12E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.93E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.34E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.12E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.53E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	5.92E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	The $Oral\ CSF$ value represents a 2,4/2,6-Dinitrotoluene mixture (U.S. EPA 1997b).	C-1-7	6.8E-01
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.5E-03
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-2-2	6.8E-01

Note:

NA = Not applicable  
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-92

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	88.10
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	284.9
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b)	--	5.00E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	9.00E+05
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.89E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.20E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.05E-05
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b)	--	5.40E-01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	8.76E-01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.76E-03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.57E-02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.50E-02
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended	B-1-1; B-2-1;	1.0

TABLE A-3-92

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.45E+00
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	7.37E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.53E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.53E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.93E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.93E-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.29E-09
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.36E-08
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.64E-08
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.29E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.07E-08

TABLE A-3-92

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.69E-01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	1.1E-02
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	3.1E-06
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-93

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	184.24
$T_m$ (K)	Montgomery and Welkom (1991)	--	401.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b)	--	4.74E-08 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	6.80E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.28E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.95E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.24E-06
$K_{ow}$ (unitless)	Montgomery and Welkom (1991)	--	8.71E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.78E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.78E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.09E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.11E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman	B-1-1; B-2-1;	0.999

TABLE A-3-93

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.90E+01
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.76E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	7.74E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	7.74E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.89E+02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.89E+02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.92E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.19E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.65E-05
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.92E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.73E-05

TABLE A-3-93

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.01E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	8.0E-01
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	2.2E-04
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	8.0E-01

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-94

## CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	274.38
$T_m$ (K)	$T_m$ value cited in U.S. EPA (1995b).	--	248
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	3.7E-07 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.6E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.12E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.50E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.21E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	9.55E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.80E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.80E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.35E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	7.20E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.20E+01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman	B-1-1; B-2-1;	0.998

TABLE A-3-94

## CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.76E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.55E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.94E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.94E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.35E+02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.35E+02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.59E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.40E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.90E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.59E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.89E-04

TABLE A-3-94

CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	6.23E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	4.00E-05
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.40E-04
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-95

## CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	406.95
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	343.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	1.72E-11 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	2.31E-01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.04E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.59E-03
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.76E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.02E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.04E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.04E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.53E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.16E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.78E+01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	0.075



TABLE A-3-95

## CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.17E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.75E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.77E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.77E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.36E+03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.36E+03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.40E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.59E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	9.18E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.40E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.99E-05

TABLE A-3-95

## CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.60E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	6.00E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.10E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-96

## CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	380.93
$T_m$ (K)	U.S.EPA (1992a)	--	473.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a)	--	7.68E-10 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a)	--	2.46E-01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.19E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.07E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	5.76E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.79E+04
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.08E+08
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.08E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.11E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.32E+02
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+04
$F_v$ (unitless)	--	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	ND

TABLE A-3-96

## CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent	B-2-10	1.36E+03
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.26E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.76E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.76E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	7.62E+03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	7.62E+03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.19E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.96E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.37E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.19E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.55E-03
$BCF_{fish}$ (L/kg, FW tissue)	--	B-4-26	NA

TABLE A-3-96

## CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

Parameter	Reference and Explanation	Equations	Value
$BAF_{fish}$ (L/kg FW)	<i>BAFs</i> were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). <i>BAF</i> values were predicted values calculated by multiplying a food chain multiplier ( <i>FCM</i> ) with an estimated <i>BCF</i> . <i>BCFs</i> were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). <i>FCMs</i> were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	8.55E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.00E-04
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.10E-03
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-97

## CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (106-89-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	92.53
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	247.5
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	2.20E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	6.60E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.08E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.13E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.10E-05
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.78E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.22E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.22E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.66E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.88E-02
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended	B-1-1; B-2-1;	1.0



TABLE A-3-97

## CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (106-89-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.67E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.00E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.77E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.77E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.35E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.35E-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.41E-08
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.47E-08
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	5.41E-08
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.41E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.53E-08



TABLE A-3-97

## CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (106-89-8)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	9.13E-01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1995b)	C-1-8	2.00E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	9.90E-03
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	1.00E-03
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	1.20E-06
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	4.20E-03

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-98

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	$MW$ value cited in U.S. EPA (1995b)	--	114.14
$T_m$ (K)	--	--	NA
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	2.30E-02 at 25°C
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.90E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.38E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.07E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.35E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.89E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.46E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.46E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.85E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	9.80E-01

TABLE A-3-98

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value cited in NC DEHNR (1997).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.02E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	4.14E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.67E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.67E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.00E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.00E-02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.09E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	9.77E-07

TABLE A-3-98

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

Parameter	Reference and Explanation	Equations	Value
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.18E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.09E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	7.71E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	9.51E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	9.00E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.20E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable  
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-99

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	124.15
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	373.0
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	3.50E-04 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	4.90E+05
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.87E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.63E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.84E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.12E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.55E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.55E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.16E-01

TABLE A-3-99

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.19E-02
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.88E+01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.56E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	4.24E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.63E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.63E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	7.11E-01

TABLE A-3-99

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ ( $\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}$ )	$Bv_{leafyveg}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	7.11E-01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	8.90E-09
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2..81E-08
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	3.41E-08
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	8.90E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	2.22E-08
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	6.42E-01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-1-7	2.93E+02
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ ( $\mu\text{g/m}^3$ ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	8.4E+01
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	2.93E+02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-100

## CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.26E-02 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.73E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.73E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.65E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.49E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.33E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.04E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.04E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.53E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.16E+00
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	2.53E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	1.0

TABLE A-3-100

## CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.52E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.20E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.07E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.07E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.53E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.53E-02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.05E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.33E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.03E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.05E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.63E-05

TABLE A-3-100

## CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.39E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	1.00E+00
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.